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Project Title: A Design Methodology for Mica Based Compressive Seals

I. Mission Statement

To develop an effective computational leakage model for mica-based compressive seals in planar solid-oxide fuel cell (SOFC) applications.

II. Technical Approach

A computational leakage model is being refined to accurately predict flow in a compressive seal assembly. A secondary objective of the leakage model will be to evaluate the validity and effectiveness of two micro contact models (e.g., the Greenwood -Williamson and Jackson-Streator model) while varying the applied compressive load, interfacial surface roughness and temperature. Before modeling a mica-based compressive seal assembly, which includes several interfaces and components, proof-of--concept leakage studies were performed on a single interface metal-metal compressive seal. An Inconel annulus is preloaded on a stainless steel substrate. A synopsis of the conditions maintained in the initial battery of metal-metal compressive seal leakage tests is included in Table 1. Each combination or row was performed three times. As indicated in Table 1, the stainless steel surface was lapped using 100 grit and 600 grit tool.

Table 1: Summary of leakage experiments conducted.

Sample	S_y (psi)	Temp (C)
100 ugrit	100	25
	300	
	500	
	100	250
	300	
	500	
	100	500
	300	
	500	
600 ugrit	100	25
	300	
	500	
	100	250
	300	
	500	
	100	500
	300	
	500	

The surface roughness results including the root mean square roughness, S_q, and maximum asperity height within the annular region, c_{max}, are included in Table 2.

Table 2: Summary of surface roughness characteristics for the two stainless steel surface finishes.

Sample	S_q (μm)	c_{max} (μm)
100 grit	22.96	109.94
600 grit	1.54	7.53

Leakage results from the above experiments were determined for subsequent comparison with leakage model predictions. Leakage model results discussed all occur in an isothermal, steady flow environment. The loading and flow conditions considered in each parametric study are identical to the conditions used in the metal-metal compressive leakage experiments presented subsequently for comparative purposes. Leakage results were obtained using the Fast Fourier Transform based Jackson-Streator model[1]. A more detailed explanation of the modeling approach and leakage submodels may be found in Green and et al[2]. An expression for the volumetric leakage rate, Q, based on mixed lubrication theory was derived and is included as follows:

$$Q = \frac{-\pi p_o^2\left(1-\left(\frac{p_i}{p_o}\right)^2\right)}{12\mu RT\int_{r_i}^{r_o}\frac{dr'}{\phi(r')r'h^3(r')}} \tag{1}$$

where p_o is the absolute pressure of the gas at the outer radius, p_i is the absolute pressure of the gas at the inner radius, μ is he kinematic viscosity, R is the gas constant for the ideal gas, and T is the absolute temperature of the gas.

A schematic of the metal-metal compressive seal assembly used throughout this preliminary study is depicted in Fig. 1. Moreover, this configuration was investigated primarily to isolate the effect surface roughness, temperature, and applied compressive load would have on leakage rates at a single interface. Since conventional mica compressive seals have multiple leakage paths as well as subcomponents with sophisticated microstructure, findings from the current study are being used to refine the aforementioned computational leakage contact model so that leakage may be accurately quantified at multiple interfaces.

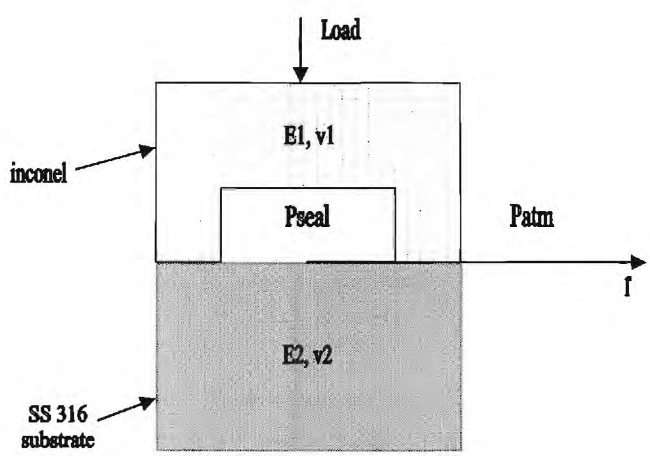

Figure 1: Depiction of metal-metal compressive seal.

The experimental setup, shown schematically in Fig. 2, was modeled after leakage experiments by Chou and Stevenson [3]. Stainless steel test specimens were lapped using 100 μgrit and 600 μgrit work pieces, respectively. The compressive load was applied using a mechanical tester with constant load control. A cylindrical reservoir of 300 cm^3 is kept at ambient conditions and is connected to the Inconel tube via a 6.35 mm stainless steel tube. The cylindrical reservoir is evacuated using a vacuum pump, and then is pressurized. A differential pressure gauge is then used to monitor the change in pressure, which is directly proportional to the instantaneous volumetric leakage rate. By assuming the Ideal Gas law, the volumetric leakage rate, L, is determined using the equation:

$$L = \frac{V_{cyl}}{\rho RT} \frac{dp}{dt} \tag{2}$$

where V_{cyl} is the reservoir volume, R_{gas} is the gas constant for the fluid, T is the temperature, and dp is the differential change in pressure, and dt is the differential change in time.

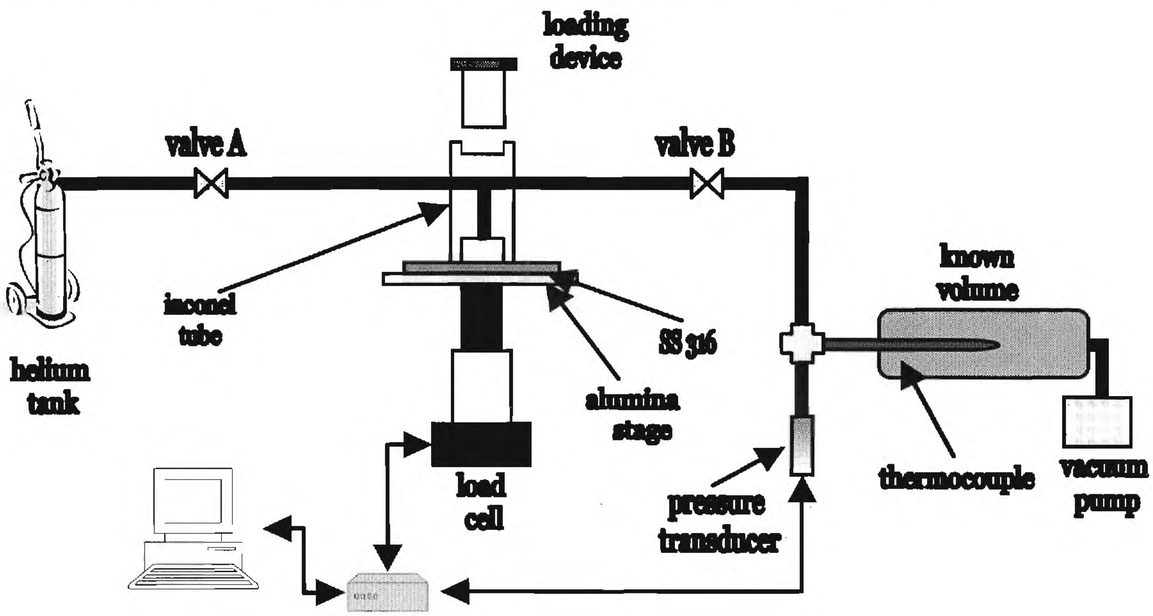

Figure 2: Schematic of experimental leakage setup.

III. Technical Results

A comprehensive metal-metal compressive seal leakage study was conducted. The modeling results were determined as follows. After the applied compressive load and ambient temperature was prescribed according to Table 1, the macro-contact model was used to determine the pressure distribution. Figure 3 shows the pressure distribution in the contact zone. From the figure, it follows that the nodal pressure values are highest at the inner and outer radii of the annulus. The behavior of the pressure profile at these two locations indicates the presence of stress concentrations due to infinitely sharp corners.

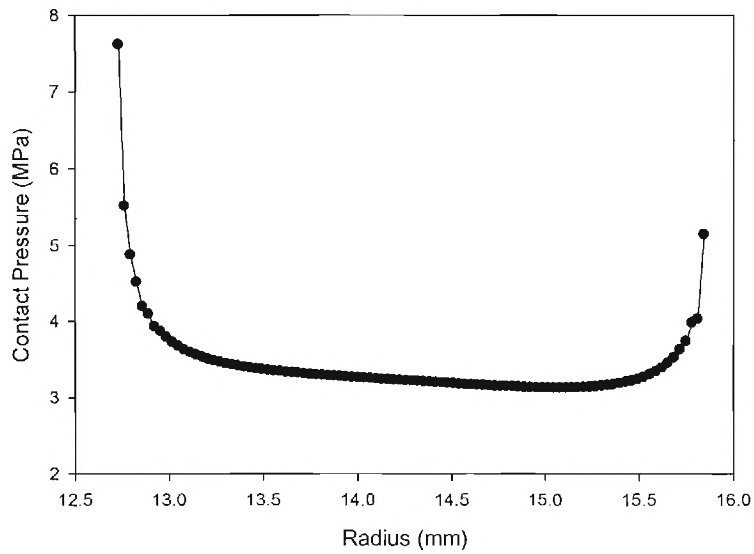

Figure 3: Pressure distribution of metal-metal compressive seal with σ= 500 psi and T_f= 25 °C.

From the micro contact model, a relationship is established between the local pressure and the average nodal surface separation is established. The normalized surface separation is then determined by dividing the local surface separation by the root mean square roughness. A representative plot of the normalized surface separation as a function of radius is included as Figure 4.

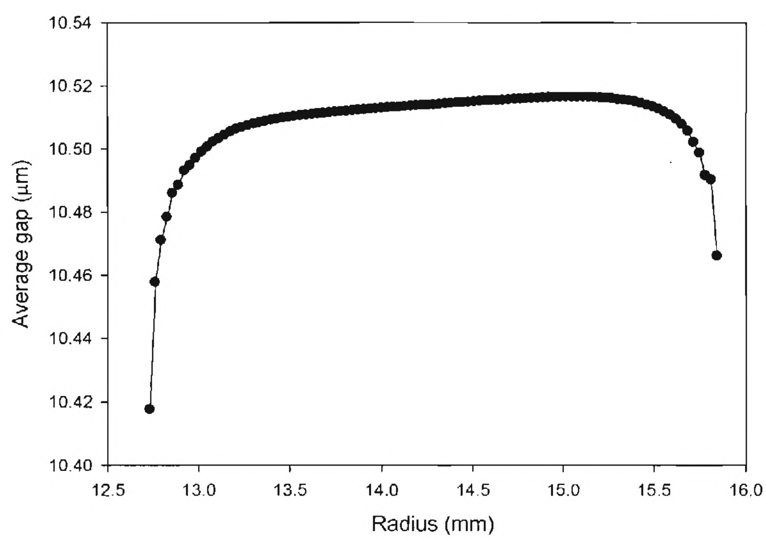

Figure 4: Normalized nodal surface separation with σ= 500 psi and T_f= 25 °C in 100 grit SS316 substrate.

As indicated in Figure 4, the normalized surface separation is the least at the edges corresponding to the inner and outer radius. At the interior nodes, the said separation seems to remain close to 10.51 microns for the 100 grit metal compressive seal specimen. The radial variation across the annular contact region was less than 1 percent.

Using the mixed lubrication model, the volumetric flow rate was determined as a function of compressive stress, surface roughness, and temperature. A synopsis of the leakage results for this metal-metal compressive seal study is included as Figures 5 and 6, respectively.

Table 3: Leakage results for metal-metal compressive seal with two surface finish variations.

Stress(psi)	Temp (C)	100 grit avg (sccm/cm)	100 grit std (sccm/cm)	600 grit avg (sccm/cm)	600 μgrit std (sccm/cm)
100	25	0.706	0.028	0.367	0.024
300	25	0.616	0.016	0.363	0.039
500	25	0.588	0.060	0.289	0.083
100	250	1.696	0.424	0.248	0.077
300	250	1.395	0.795	0.220	0.076
500	250	1.143	0.311	0.204	0.064
100	500	1.270	0.319	0.199	0.068
300	500	0.886	0.185	0.203	0.080
500	500	0.962	0.062	0.210	0.073

Table 4: Computational model leakage predictions for metal-metal compressive seal assembly.

Stress(psi)	Temp, C	100 grit (sccm/cm)	600 grit (sccm/cm)
100	25	1740.267	0.558
300	25	1739.643	0.555
500	25	1739.022	0.552
100	250	1183.786	0.231
300	250	1183.513	0.231
500	250	1183.240	0.231
100	500	888.177	0.218
300	500	888.040	0.218
500	500	888.040	0.218

By comparing the average leakage rate results in Table 3 to the model predictions in Table 4, it follows that in general the computational model over predicts the leakage experiment results. The 100 grit leakage model results are significantly higher than its experimental counterpart, whereas the 600 grit model predictions are either within or close to the experimental error band for all cases.

The computational model was reasonably effective in predicting the leakage rates in the 600 grit compressive seal assembly. According to Fig. 5, which shows the effect of compressive load for 25°C with the 100 grit sample the both models (elastic and elastic-plastic) over-predict the leakage as compared to the experimental results. Figure 6 shows slightly better agreement for the 600 grit case.

Figures 7 & 8 show results for conditions like those of Figs. 5 & 6, but with the temperature at 500°C. In Fig. 7, we see that, again for the 600 grit case, both models over-predict the leakage results. In Fig. 8, both models show a little better agreement, with the elastic-plastic predictions either falling within the experimental error bars at the two lower loads, and the elastic only model falling just outside of the error bars at the lower loads. Overall, the computational model performs reasonably well for the smoother surface.

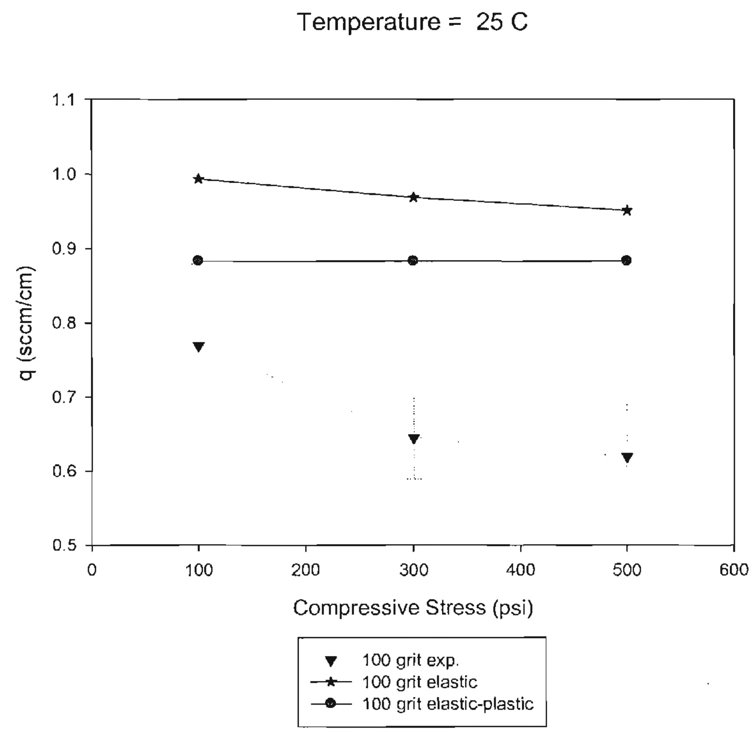

Figure 5: Graphical comparison of volumetric leakage rate per seal length as a function of compressive stress for Inconel/ 100 grit SS 316 compressive seal at 2 kPa (0.29 psig) with Temperature = 25 °C.

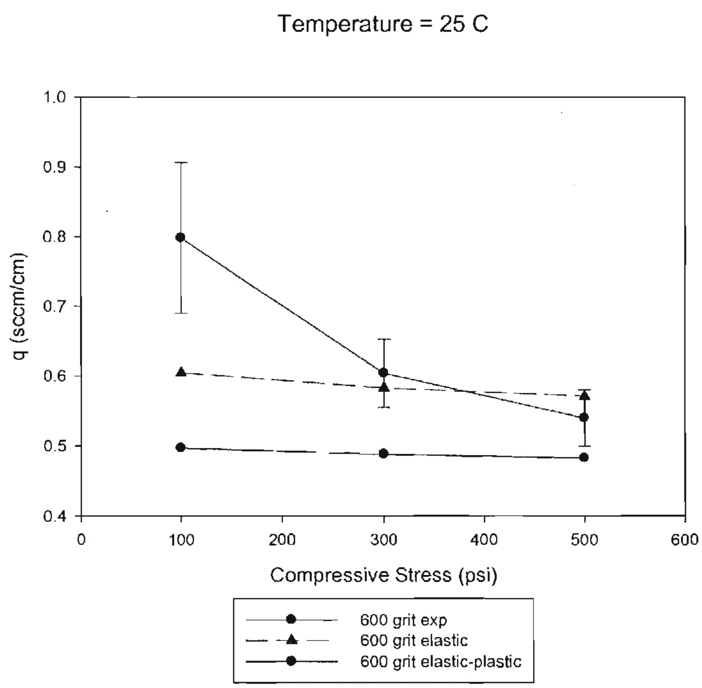

Figure 6: Graphical comparison of volumetric leakage rate per seal length as a function of compressive stress for Inconel/ 600 grit SS 316 compressive seal at 2 kPa (0.29 psig) with Temperature = 25 °C.

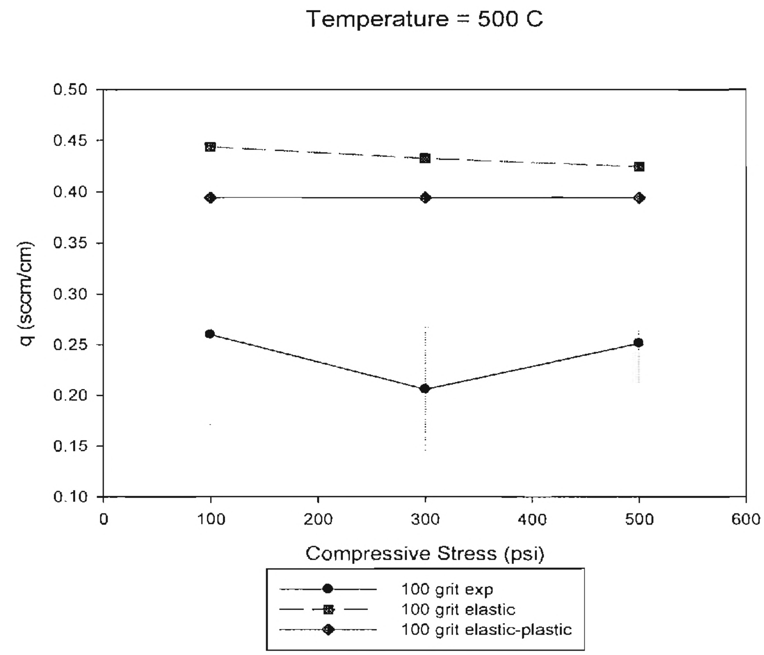

Figure 7: Graphical comparison of volumetric leakage rate per seal length as a function of compressive stress for Inconel/ 100 grit SS 316 compressive seal at 2 kPa (0.29 psig) with Temperature = 500 °C.

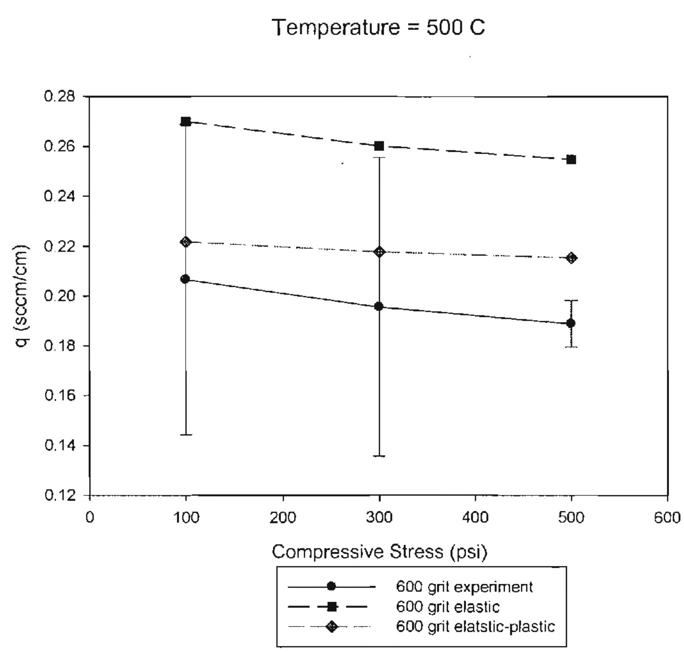

Figure 8: Graphical comparison of volumetric leakage rate per seal length as a function of compressive stress for Inconel/ 600 grit SS 316 compressive seal at 2 kPa (0.29 psig) with Temperature = 500 °C.

IV. Accomplishments for the TTRF Project

- Experimental apparatus was developed at Oak Ridge National Laboratories (Oak Ridge, TN) for testing leakage of annular compressive seals under controlled temperature conditions.
- A computational model of compressive seal leakage was developed based on a combination of (1) finite element macro-contact model, (2) a 3D multi-scale micro-contact model, and (3) a compressible- fluid, mixed-lubrication flow model.
- A Ph.D. student (Christopher Green) successfully presented his Ph.D. Dissertation Proposal: "Development of Leakage Model for Solid Oxide Fuel Cell Compressive Seals."
- A research paper based on this project was presented by graduate student (Christopher Green) at the International Mechanical Engineering Conference and Exposition 2006, Chicago , IL, November 5-10, 2006.
- Results of work was presented by C. Green at the Fifth International Fuel Cell Science, Engineering, and Technology Conference, June 18-20, 2007, New York, NY.
- A research paper based on this project was accepted at the Fuel Cell Science, Engineering, and Technology Journal.
- Work from the project was presented C. Green at the 34th LEEDS LYON Symposium, Lyon, France, 4th - 7th September 2007.
- A research paper based on this project was submitted to the Tribology International journal.
- An extended abstract entitle "Leakage Studies with Seals for Solid Oxide Fuel Cells," was accepted for presentation at the 2007 International Joint Tribology Conference, October 22-24, San Diego, CA,

V. Publications

1. C. K. Green, J. L. Streator, and C. Haynes, 2006, "Modeling Leakage with Mica-Based Compressive Seals For Solid Oxide Fuel Cells," Proceedings of IMECE2006, Chicago, IL, November 5-10 2006.
2. C. K. Green, J. L. Streator, C. Haynes, and E. Lara-Curzio 2007, "A Computational Leakage Model for Solid Oxide Fuel Cell Compressive Seals," Journal of Fuel Cell Science, Engineering and Technology, accepted.
3. C. K. Green, J. L. Streator, C. Haynes, and E. Lara-Curzio 2007, "Leakage Studies with Metal-Metal Compressive Seals for Solid Oxide Fuel Cells," Tribology International, submitted.

VI. References Cited

[1] R. L. Jackson and J. L. Streator, "A multi-scale model for contact between rough surfaces," *Wear*, vol. 261, pp. 1337-1347, 2006.

[2] C. K. Green, J. L. Streator, and C. Haynes, "Modeling Leakage with Mica-Based Compressive Seals For Solid Oxide Fuel Cells," presented at International Mechanical Engineering Conference and Exposition 2006, Chicago , IL, 2006.

[3] Y.-S. Chou and J. W. Stevenson, "Thermal cycling and degradation mechanisms of compressive mica-based seals for solid oxide fuel cells," *Journal of Power Sources*, vol. 112, pp. 376-83, 2002.